Notes for Lecture 13

Fermi gas

Here we continue our exploration of the quantum ideal gas. We will study the quantum regime, where fermions (and bosons) show their truly peculiar and fascinating behaviors.

13.1 Fermi gas

Although this model sounds very naive, it is actually one of the most important models for the theory of electrons in metals and certain quantum liquids such as ^{3}He. The importance of this model is that the so-called Landau Fermi liquid is defined as a quantum liquid whose elementary particles can be mapped to free fermions in a Fermi gas.

13.1.1 Sommerfeld expansion

Let us start by stating this important expansion

$$\begin{aligned}\int_{-\infty}^{\infty} H(\varepsilon) f(\varepsilon) d\varepsilon \;&=\; \int_{-\infty}^{\mu} H(\varepsilon) d\varepsilon + \frac{\pi^2}{6} H'(\mu)(k_B T)^2 \\ &+\; \frac{7\pi^2}{360} H'''(\mu)(k_B T)^4 + O\left(\frac{T}{T_F}\right)^6 \end{aligned} \tag{13.1}$$

where $f(\varepsilon)$ is the Fermi-Dirac function[1] and $H(\varepsilon)$ is a function such that its integral ($K(\varepsilon) \equiv \int_{-\infty}^{\varepsilon} dy H(y)$) satisfies the properties that $K(-\infty) = 0$ and $K(\varepsilon)e^{-\beta\varepsilon} \to 0$ as $\varepsilon \to \infty$.

The assumption of this expansion is that

$$\frac{T}{T_F} \ll 1 \tag{13.2}$$

where T_F is the so-called *Fermi temperature*, which we will identify shortly. At this point, it suffices to know that this expansion is valid in the quantum degenerate regime, low T or high n.

The reason that the Sommerfeld expansion works is because $-f'(\varepsilon)$ is a sharply peaked function[2] at $\varepsilon = \mu$ with a unit area (if $T \ll T_F$) and it converges to a Dirac delta function, $\delta(\varepsilon - \mu(T = 0))$, in the limit of T/T_F going to zero. Note that $\mu(T = 0) \equiv \varepsilon_F \equiv k_B T_F$, where ε_F is the so-called *Fermi energy*.

The reason that the perturbation parameter is T/T_F will become clearer as we go along. However, even now, one can note the following. In the order of magnitude, $H'(\mu) \sim H(\mu)/\mu$ and so the order of the magnitude for the second term is $H\mu(k_B T/\mu)^2$. Similarly the fourth order term is of order $H\mu(k_B T/\mu)^4$. So, it is clear that the perturbation parameter is $k_B T/\mu \approx T/T_F$, if $\mu \approx \varepsilon_F = k_B T_F$. We will see shortly that indeed the chemical potential μ is equal to its zero temperature value $k_B T_F$ with a small 2nd order correction.

Once we identify the nature of $-f'(\varepsilon)$, the Sommerfeld expansion follows rather easily.

$$\int_{-\infty}^{\infty} H(\varepsilon) f(\varepsilon) d\varepsilon = K(\varepsilon) f(\varepsilon)|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} K(\varepsilon) f'(\varepsilon) d\varepsilon \tag{13.3}$$

$$= -\int_{-\infty}^{\infty} K(\varepsilon) f'(\varepsilon) d\varepsilon \tag{13.4}$$

due to the assumptions made on $K(\varepsilon)$. Since $-f'(\varepsilon)$ is peaked around $x \equiv \varepsilon - \mu = 0$, we can expand $K(\varepsilon)$ as a power series of x. Noting that $-f'(\varepsilon)$ is an even function of x, we see that odd power terms vanish when integrated with $-f'(\varepsilon)$. So, we get

$$\int_{-\infty}^{\infty} H(\varepsilon) f(\varepsilon) d\varepsilon \approx -\int_{-\infty}^{\infty} d\varepsilon K(\mu) f'(\varepsilon) - \int_{-\infty}^{\infty} d\varepsilon \frac{K''(\mu)}{2} (\varepsilon - \mu)^2 f'(\varepsilon)$$

$$= K(\mu) + 2H'(\mu)(k_B T)^2 \int_0^{\infty} dy \frac{y}{e^y + 1} \tag{13.5}$$

[1] Note that here, we expand the range of ε to $-\infty$, even if the physical spectrum is bounded from below, like $\varepsilon \geq 0$. The reason is the mathematical convenience. Since $f'(\varepsilon)$ is exponentially small at the minimum value of the physical energy spectrum if $T \ll T_F$, it introduces practically no error, essentially, if we extend $f(\varepsilon)$ to $\varepsilon \to -\infty$, since the introduced error is exponentially small.

[2] Its FWHM is about $4k_B T$.

where in the last step, three things are done concurrently: the variable substitution $y \equiv \beta(\varepsilon - \mu)$, noting the symmetry of the integral and halving the integral range with the introduction of an overall factor of 2, and the integration by parts. The integral is $\pi^2/12$ and thus the Sommerfeld expansion, Eq. 13.1, is proven to the $(T/T_F)^2$ order. This expansion can be carried out more systematically and coefficients for all orders can, in fact, be written down in a closed form, but in practice we hardly need more than what we just derived. The fourth order term is written above in Eq. 13.1, really just for information.

13.1.2 Chemical potential

We use Eq. 12.30 to figure out the chemical potential. We have, after extending the density of states to $\varepsilon = (-\infty, \infty)$ by defining $D(\varepsilon) = 0$ for $\varepsilon < 0$ or the minimum of the physical energy spectrum,

$$N = \int_{-\infty}^{\infty} d\varepsilon D(\varepsilon) f(\varepsilon) \tag{13.6}$$

$$\approx \int_{-\infty}^{\mu} d\varepsilon D(\varepsilon) + \frac{\pi^2}{6} D'(\mu)(k_B T)^2 \qquad \text{Eq. 13.1} \tag{13.7}$$

$$= N + \int_{\varepsilon_F}^{\mu} d\varepsilon D(\varepsilon) + \frac{\pi^2}{6} D'(\mu)(k_B T)^2 \qquad \text{using } \int_{-\infty}^{\varepsilon_F} d\varepsilon D(\varepsilon) = N \tag{13.8}$$

$$\approx N + (\mu - \varepsilon_F) D(\varepsilon_F) + \frac{\pi^2}{6} D'(\varepsilon_F)(k_B T)^2 \qquad \text{assuming } \mu \approx \varepsilon_F \tag{13.9}$$

Thus, we get

$$\mu \approx \varepsilon_F - \frac{\pi^2}{6} \frac{D'(\varepsilon_F)}{D(\varepsilon_F)} (k_B T)^2 \tag{13.10}$$

which justifies the assumption that $\mu \approx \varepsilon_F$ if $T \ll T_F$.

13.1.3 Fermi energy

The Fermi energy is an important energy scale of the Fermi gas problem. If one divides it by k_B, then one gets the temperature scale T_F. This temperature is the crossover temperature above which the system will behave as a classical system. If $T \ll T_F$, then the system acts as a quantum system. In the quantum system, the energy per particle is about ε_F. It is one of the most striking consequences of the Pauli exclusion principle that even at $T = 0$ the Fermi gas system imparts such a high energy to each particle. For this reason, many properties of the Fermi gas system is essentially a $T = 0$ property: e.g., the pressure, the energy, and the compressibility.

Since the free electrons in a metal bind the material together ("metallic bonding"), really the existence of a metallic substance and the reason why it hurts when you kick a metal pole are all due to the $T = 0$ quantum effect of the electron gas in the metallic substance. In this sense, any metallic substance that you see around yourself should be viewed as a quantum matter.

It is plain to see why T_F for a common metal is easily as high as $10,000$ K or $100,000$ K. First of all, note that k_F, the *Fermi wave vector* or the *Fermi momentum* (with $\hbar$ implicitly multiplying to it)—the maximum value of the magnitude of the momentum for occupied states at $T = 0$—is determined by the equation:

$$2\frac{\frac{4\pi}{3}k_F^3}{\frac{8\pi^3}{V}} = N \tag{13.11}$$

where 2 is from the spin degeneracy of the electron. So

$$k_F = \sqrt[3]{3\pi^2 n} \tag{13.12}$$

Since $n \sim 10^{-1}\text{Å}^{-3}$ for a typical metal, we get $k_F \sim 1$ to 2 Å^{-1}. For a non-relativistic electron, we then get

$$\varepsilon_F = \frac{\hbar^2}{2m}k_F^2 = 4 \sim 16 \text{ eV} \tag{13.13}$$

which definitely justifies the assumption of the non-relativistic electron. Using $k_B = 0.02585$ meV/300 K we get

$$T_F = 10,000 \text{ K} \sim 100,000 \text{ K} \tag{13.14}$$

This is the temperature scale corresponding to the typical kinetic energy of the electron in a Fermi gas at $T = 0$.

The Fermi gas problem is important not only for the electron gas in a metal, but for electrons and nucleons in a star or liquid of ^{3}He. The Fermi temperature can range from 10^6 K to a few mK, depending on systems.

13.1.4 Energy and heat capacity

Let us calculate the energy using

$$E = \int_{-\infty}^{\infty} d\varepsilon\, \varepsilon D(\varepsilon) f(\varepsilon) \tag{13.15}$$

$$\approx \int_{-\infty}^{\mu} d\varepsilon\, \varepsilon D(\varepsilon) + \frac{\pi^2}{6}\left(D(\mu) + \mu D'(\mu)\right)(k_B T)^2 \quad \text{Eq. 13.1} \tag{13.16}$$

$$= E_0 + \int_{\varepsilon_F}^{\mu} d\varepsilon\, \varepsilon D(\varepsilon) + \frac{\pi^2}{6}\left(D(\mu) + \mu D'(\mu)\right)(k_B T)^2 \quad E_0 \equiv \int_{-\infty}^{\varepsilon} d\varepsilon\, \varepsilon_F D(\varepsilon) \tag{13.17}$$

Using the result, Eq. 13.10, we see that $\int_{\varepsilon_F}^{\mu} d\varepsilon\, \varepsilon D(\varepsilon) \approx -\frac{\pi^2}{6}\mu D'(\mu)(k_B T)^2$ cancels one of the terms above, and we have finally (with $\mu \approx \varepsilon_F$)

$$E \approx E_0 + \frac{\pi^2}{6} D(\varepsilon_F)(k_B T)^2 \tag{13.18}$$

The heat capacity is

$$C_V \approx \frac{\pi^2}{3} D(\varepsilon_F)(k_B T) k_B \tag{13.19}$$

These expressions have a very precise qualitative interpretation. With respect to the ground state ("vacuum") at $T = 0$, a finite temperature state is characterized by the electrons excited above μ and the holes[3] excited below μ. Mathematically the presence of these excitations is indicated by the fact that $f(\varepsilon, T)$ deviates from $f(\varepsilon, T = 0)$. Since this deviation occurs in a small sliver of energy of width about $4k_B T$, we can estimate that the number of electrons and holes excited around the chemical potential are given by $\sim D(\varepsilon_F)(k_B T)$. These are particles whose energy relative to the $T = 0$ "vacuum" is less than the temperature—i.e., they act as classical particles with equipartition energy $\sim k_B T$ per particle. This is the reason why $E \sim D(\varepsilon_F)(k_B T)(k_B T)$ up to a numerical factor, and why $C_V \sim D(\varepsilon_F)(k_B T)k_B$ up to a numerical factor.

13.1.5 Order of magnitude and dispersion

As we have been doing the 2nd order perturbation on T/T_F, we expect that $E_0 \gg E - E_0$ and likewise $P_0 \gg P - P_0$ (cf. Eq. 12.32). That this is really true can be analyzed as follows. $D(\varepsilon_F) \sim N/\varepsilon_F$. $E_0 \sim N\varepsilon_F$. And so, from Eq. 13.18, we get $E - E_0 \sim E_0(T/T_F)^2 \ll E_0$.

Purposefully, we did not specify the nature of the Fermion so much in this note so far (with the exception of Section 13.1.3). This leaves all expressions so far applicable regardless of relativistic or non-relativistic particles and the dimensionality of the space.

Here, we take up the non-relativistic case in three dimensions as we did in Section 13.1.3. Note that in this case the density of states is proportional to $\varepsilon^{1/2}$ (Eq. 12.45). Thus, by setting $D(\varepsilon) = A\varepsilon^{1/2}$ and using $\int_0^{\varepsilon_F} d\varepsilon D(\varepsilon) = N$ (the zero temperature particle conservation equation), we get

$$D(\varepsilon) = \frac{3}{2}\frac{N}{\varepsilon_F}\left(\frac{\varepsilon}{\varepsilon_F}\right)^{1/2} \tag{13.20}$$

[3]These holes are somewhat different from holes in semiconductors, and should not be confused with them.

Comparing this expression with Eq. 12.45 gives another way to evaluate ε_F in terms of the system parameters. From this expression, it is readily found that

$$E_0 \equiv E(T=0) \;=\; \int_0^{\varepsilon_F} d\varepsilon\, \varepsilon D(\varepsilon) \;=\; \frac{3}{5} N \varepsilon_F \tag{13.21}$$

which means

$$P(T=0)V \;=\; \frac{2}{5} N \varepsilon_F \tag{13.22}$$

Also, we get

$$D(\varepsilon_F) \;=\; \frac{3}{2}\frac{N}{\varepsilon_F} \tag{13.23}$$

$$\frac{D'(\varepsilon_F)}{D(\varepsilon_F)} \;=\; \frac{1}{2}\frac{1}{\varepsilon_F} \tag{13.24}$$

and therefore

$$\mu \;=\; \varepsilon_F \left(1 - \frac{\pi^2}{12}\left(\frac{T}{T_F}\right)^2 + O\left(\frac{T}{T_F}\right)^4\right) \tag{13.25}$$

$$E \;=\; \frac{3}{5} N \varepsilon_F \left(1 + \frac{5\pi^2}{12}\left(\frac{T}{T_F}\right)^2 + O\left(\frac{T}{T_F}\right)^4\right) \tag{13.26}$$

$$C_V \;=\; \frac{\pi^2}{2} N k_B \frac{T}{T_F} + O\left(\frac{T}{T_F}\right)^3 \tag{13.27}$$

13.1.6 Heavy fermion

The heat capacity for a free fermion system is typically written as

$$C_V \;=\; \gamma T \tag{13.28}$$

where according to Eq. 13.19

$$\gamma \;=\; \frac{\pi^2}{3} D(\varepsilon_F) k_B^2 \tag{13.29}$$

Here, γ has the dimension of mJ / mole / K^2. For a typical metal, it has the value of $\gamma \sim 1$ mJ / mole / K^2. However, for certain materials called "heavy fermions" (e.g. UPt_3, UBe_{13}, $CeCu_2Si_2$, ...), γ can be as large as 1000! It is as though an electron is as heavy as a neutron! To explain this one notes that $\gamma \propto m$, since $D(\varepsilon_F) \sim N/\varepsilon_F$ and $\varepsilon_F \propto 1/m$. It turns out that what we call "free fermions" are sometimes collective particles that emerge out of very strong interactions. Those particles are called "renormalized particles" or "quasi-particles." In the heavy fermion

case, these quasi-particles act just like free electrons except that each heavy fermion, i.e. each quasi-particle, has a very large mass. In this case, the heavy mass originates from the Kondo interaction—the spin-flip scattering of a conduction electron off of a spin impurity. This problem cannot be solved perturbatively and has been vexing physicists for years, before it was masterfully solved by K. G. Wilson.